1,3-Benzodioxole-5-methanol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 69.5 °C

Global applicability domain: Inside

Local applicability domain index: 6.36e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

Image not found
1,3-Benzodioxole-5-methanol
Measured: 58.0
Predicted: 69.5

Image not found
4-Hydroxy-3-methoxybenzaldehyde
Measured: 81.5
Predicted: 94.6

Image not found
3-Hydroxy-4-methoxy-benzaldehyde
Measured: 114
Predicted: 97.7

Image not found
4-Hydroxy-3-methoxycinnamaldehyde
Measured: 84.0
Predicted: 99.0

Image not found
3-Ethoxy-4-hydroxybenzaldehyde
Measured: 77.5
Predicted: 92.7